#### MPI on the Grid

#### William Gropp

Mathematics and Computer Science Argonne National Laboratory http://www.mcs.anl.gov/~gropp With help from Rusty Lusk, Nick Karonis



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#### **Outline**

- Why MPI?
- MPI Point-to-point communication
- MPI Collective communication
- Performance and Debugging
- MPICHG2

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### Why use MPI on the Grid?

- Applications already exist
- Tools exist
  - Libraries and components, some enabled for the Grid
    - E.g., Cactus (Gordon Bell winner)
- Simplifies Development
  - ◆ "Build locally, run globally"
  - ♦ NSF TeraGrid plans this approach

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## Why use the MPI API on the Grid?

- MPI's design is latency tolerant
- Separation of concerns matches the needs of Grid infrastructure
  - ♦ MPI itself has no "grid awareness"
  - MPI designed to operate in many environments
    - The Grid is "just" another such environment

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## Specification and Implementation

- MPI is a specification, not a particular implementation
- MPI (the specification) has many features that make it well-suited for Grid computing
- There are many opportunities for enhancing MPI implementations for use in Grid computing
  - Some tools already exist
  - Great opportunities for research and papers for EuroPVMMPI'03!

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#### Grid Issues

- Simplest "grid" model
  - Multiple systems that do not share all resources
    - Example: Several clusters, each with its own file system
- More complex model
  - Multiple systems in separate administrative domains
    - Example: Several clusters, each administered by a different organization, with different access policies and resources
- · (Mostly) Shared Properties
  - Geographic separation
    - From 1 to 10000km
    - · Each 1000km gives at least 3ms of latency
      - Typical of disk access!
  - Process management separate from communication
    - Must not assume any particular mechanism for creating processes

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## Issues When Programming for the Grid

- Latency
  - Using MPI's send modes to hide latency
- Hierarchical Structure
  - Developing and using collective communication for high, unequal latency
- Handling Faults

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# Quick review of MPI Message passing

- Basic terms
  - nonblocking Operation does not wait for completion
  - synchronous Completion of send requires initiation (but not completion) of receive
  - ready Correct send requires a matching receive
  - asynchronous communication and computation take place simultaneously, not an MPI concept (implementations may use asynchronous methods)

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#### **Communication Modes**

- MPI provides multiple modes for sending messages:
  - Synchronous mode (MPI\_Ssend): The send does not complete until a matching receive has begun.
  - Buffered mode (MPI\_Bsend): The user supplies a buffer to the system for its use.
  - Ready mode (MPI\_Rsend): User guarantees that a matching receive has been posted.
    - · Allows access to fast protocols
    - · Undefined behavior if matching receive not posted
- Non-blocking versions (MPI\_Issend, etc.)
- MPI\_Recv receives messages sent in any mode.

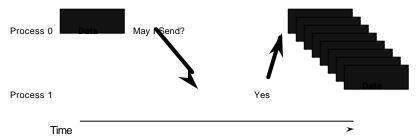
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### What is message passing?

· Data transfer plus synchronization



- Requires cooperation of sender and receiver
- Cooperation not always apparent in code

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### Message protocols

- Message consists of "envelope" and data
  - Envelope contains tag, communicator, length, source information, plus impl. private data
- Short
  - Message data (message for short) sent with envelope
- Eager
  - Message sent assuming destination can store
- Rendezvous
  - Message not sent until destination oks

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### **Eager Protocol**



Time

- Data delivered to process 1
  - No matching receive may exist; process 1 must then buffer and copy.

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#### Eager Features

- Reduces synchronization delays
- Simplifies programming (just MPI\_Send)
- Requires significant buffering
- May require active involvement of CPU to drain network at receiver's end
- May introduce additional copy (buffer to final destination)
- Minimizes latency

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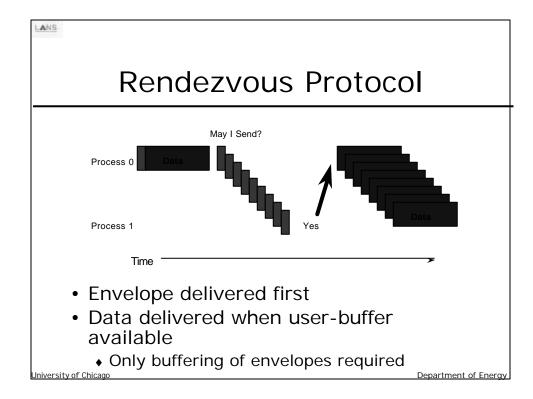
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## How Scaleable is Eager Delivery?

- Buffering must be reserved for arbitrary senders
- User-model mismatch (often expect buffering allocated entirely to "used" connections).
- Common approach in implementations is to provide same buffering for all members of MPI\_COMM\_WORLD; this is optimizing for non-scaleable computations
- Scalable implementations that exploit message patterns are possible (but not widely implemented)

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#### Rendezvous Features

- Robust and safe
  - (except for limit on the number of envelopes...)
- May remove copy (user to user direct)
- More complex programming (waits/tests)
- May introduce synchronization delays (waiting for receiver to ok send)
- Three-message handshake introduces latency

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#### **Short Protocol**

- Data is part of the envelope
- Otherwise like eager protocol
- May be performance optimization in interconnection system for short messages, particularly for networks that send fixed-length packets (or cache lines)

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### Implementing MPI\_Isend

- Simplest implementation is to always use rendezvous protocol:
  - MPI\_Isend delivers a request-to-send control message to receiver
  - Receiving process responds with an ok-to-send
    - May or may not have matching MPI receive; only needs buffer space to store incoming message
  - Sending process transfers data
- Wait for MPI\_Isend request
  - wait for ok-to-send message from receiver
  - wait for data transfer to be complete on sending side

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#### Alternatives for MPI\_Isend

- Use a short protocol for small messages
  - No need to exchange control messages
  - Need guaranteed (but small) buffer space on destination for short message envelope
  - Wait becomes a no-op
- Use eager protocol for modest sized messages
  - Still need guaranteed buffer space for both message envelope and eager data on destination
  - Avoids exchange of control messages

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### Implementing MPI\_Send

 Can't use eager always because this could overwhelm the receiving process

if (rank != 0) MPI\_Send( 100 MB of data )
else receive 100 MB from each process

- Would like to exploit the blocking nature (can wait for receive)
- · Would like to be fast
- Select protocol based on message size (and perhaps available buffer space at destination)
  - Short and/or eager for small messages
  - Rendezvous for longer messages

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### Implementing MPI\_Rsend

- Just use MPI\_Send; no advantage for users
- Use eager always (or short if small)

Even for long messages

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### Choosing MPI Alternatives

- MPI offers may ways to accomplish the same task
- Which is best?
  - Just like everything else, it depends on the vendor, system architecture, computational grid environment
  - Like C and Fortran, MPI provides the programmer with the tools to achieve high performance without sacrificing portability

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## Using MPI\_Rsend to Minimize Latency

- For high-latency environments, avoid message handshakes
  - Problem: Must guarantee that sufficient space is available at destination for the message without exchanging messages
  - Use algorithmic features and double buffering to enforce guarantees

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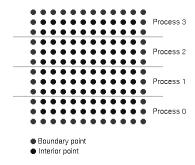
### Using MPI\_Rsend

- Illustrate with simple Jacobi example
  - Typical data motion for many applications
  - ◆ Specific numeric algorithm is obsolete

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#### Jacobi Iteration

Simple parallel data structure



Processes exchange rows with neighbors

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#### Send and Recv

- Simplest use of send and recv
- MPI\_Status status;

MPI\_Send( xlocal+m\*lrow, m, MPI\_DOUBLE, up\_nbr, 0, comm );

MPI\_Recv( xlocal, m, MPI\_DOUBLE, down\_nbr, 0, comm, &status );

MPI\_Send( xlocal+m, m, MPI\_DOUBLE, down\_nbr, 0, comm);

MPI\_Recv( xlocal+m\*(lrow+1), m, MPI\_DOUBLE,
up\_nbr, 1, comm, &status);

· Receives into ghost rows

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## What is the whole algorithm?

#### 1. Loop

- 1. Exchange ghost cells
- 2. Perform local computation (Jacobi sweep)
- 3. Compute convergence test using MPI Allreduce
- 2. Until converged

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## What is the ready-send version of the algorithm?

- Initialize (post nonblocking receives, barrier or initial MPI\_Allreduce)
- 2. Loop
  - Exchange ghost cells using MPI\_Rsend (or MPI\_Irsend)
  - 2. Perform local computation (Jacobi sweep)
  - 3. Post nonblocking receives for next iteration
  - 4. Compute convergence test using MPI\_Allreduce
- 3. Until converged
  - 1. Cancel unneeded receives with MPI\_Cancel

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#### Rsend and Irecv

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#### Recommendations

- Aggregate short messages
- Structure algorithm to use MPI\_Rsend or MPI\_Irsend
- Avoid MPI\_Ssend
- Once more MPI implementations support MPI\_THREAD\_MULTIPLE, restructure algorithms to place MPI communication into a separate thread
  - MPI\_Init\_thread is used to request a particular level of thread support; it returns as a parameter the available level of thread support

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#### Research Topics

- Reduce the number of internal messages for sending large messages
  - "Receiver rendezvous" instead of sender rendezvous
    - Difficulties with MPI\_ANY\_SOURCE might be addressed with communicator-specific attribute values
  - Adaptive allocation of buffer space (increasing eager threshold), to make Rsend approach unnecessary
  - "Infinite window" replacements for IP/TCP
    - Provide effect of multiple TCP paths but with sensible flow control and fair resource sharing

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## Using MPI Collective Operations

- Collective routines offer a simpler programming model
- Puts the burden of implementing the best communication algorithm on the MPI implementor
  - Typical implementations not optimized (see Tuesday's talk on MPICH2)
  - Few implementations are grid optimized
- I will discuss the implementation in MPICH-G2
  - Another good implementation is MagPIE (see http://www.cs.vu.nl/albatross/#software)

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#### Topology-Aware Collective Team

- Original Design and Implementation
  - ◆ Bronis R. de Supinski
  - Nicholas T. Karonis
  - Ian Foster
  - ◆ William Gropp
  - Ewing Lusk
  - ◆ John Bresnahan
- · Updated Implementation by
  - ◆ Sebastien Lacour

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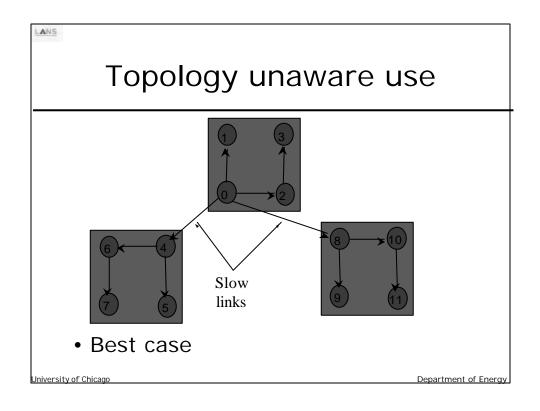
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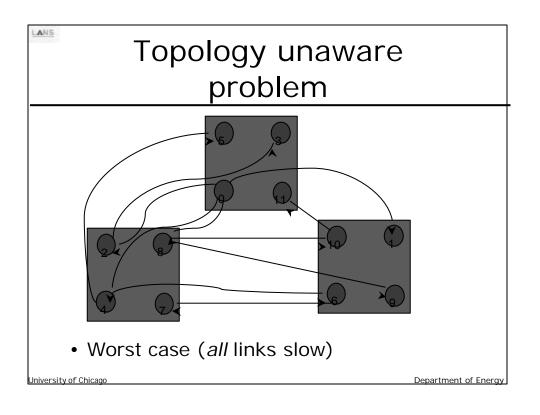
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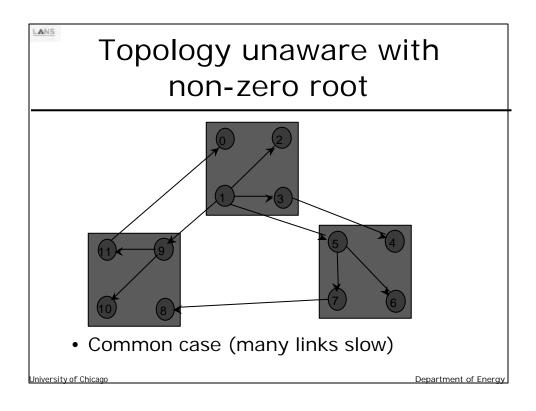
## Multi-level communication systems

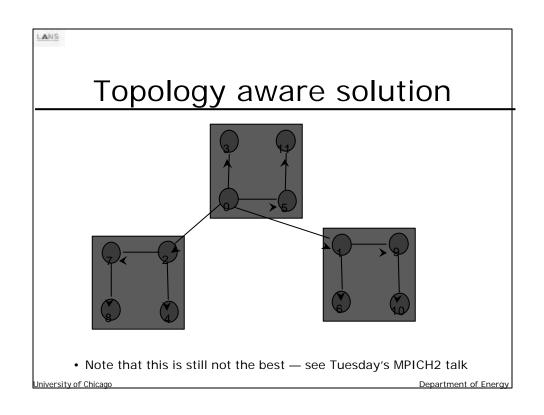
- Order(s) of magnitude performance differences
  - ◆ Latency
  - ◆ Bandwidth
- Examples
  - ◆ SMP Clusters
  - Computational grid

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## Why a Multi-Level Implementation?

- Two levels do not capture all important systems
  - Where to split multilevel system into two?
    - · Between two slowest levels?
    - · Between two fastest levels?
    - · Who determines?
- Original problem recurs at coalesced levels
- Two level approaches can degenerate to topology unaware solution for derived communicators

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### MPICH-G2 Topology Aware Implementation

- Determine topology
  - During start-up or communicator creation
  - Hidden communicators
    - Clusters
    - Masters
- Perform operation "recursively" over masters
- MPICH ADI additions
  - MPID\_Depth
  - MPID\_Clusterid

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## Hidden Communicator Creation

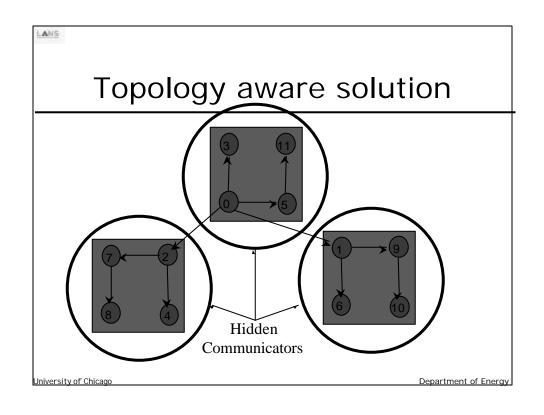
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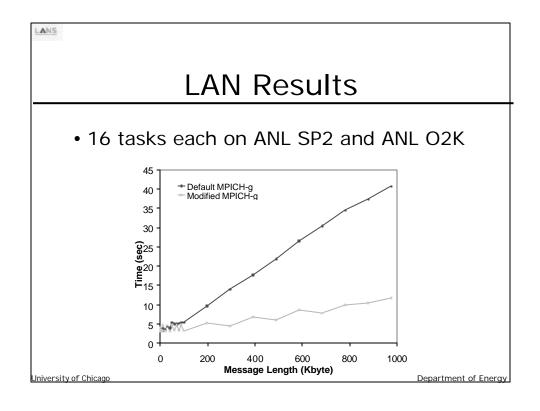
### Broadcast algorithm

Non-zero roots:

Substitute root for its master at faster levels Replace 0 with root in level broadcast if necessary

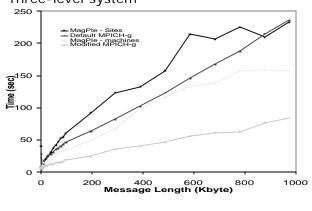
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### Comparative Performance Results

- 16 tasks each on ANL SP2, O2K and SDSC SP2
  - Three-level system



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### **Topology Information**

- MPICH-G2 exports information on system topology to applications programs through attributes:
- MPICHX\_TOPOLOGY\_DEPTHS
  - $\bullet$  Vector,  $i^{th}$  value is depth of  $i^{th}$  process
- MPICHX\_TOPOLOGY\_COLORS
  - Vector of pointers to arrays; the i<sup>th</sup> vector has length corresponding to the depth of that process and the values are the color at that level

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## Accessing Topology Information in MPICH-G2

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### Performance and Debugging Tools

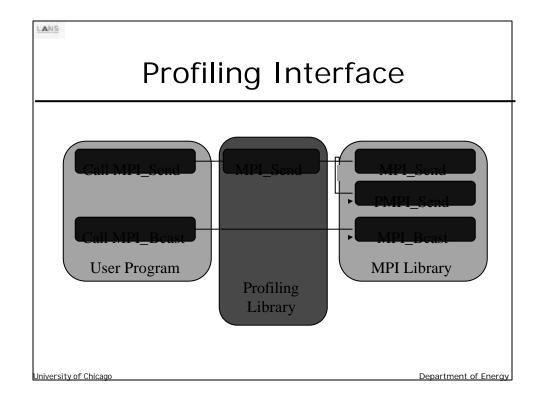
- Not a pretty picture
- No real grid debuggers
- Few application-level performance tools
- MPI provides a powerful hook on which to build customized performance and correctness debugging tools

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### Using PMPI routines

- PMPI allows selective replacement of MPI routines at link time (no need to recompile)
- Some libraries already make use of PMPI
- Some MPI implementations have PMPI bugs
  - PMPI may be in a separate library that some installations have not installed

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## Using the Profiling Interface

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### Collecting Data From the Profiling Interface

 Use MPI\_Finalize to force each process to either collect data (using MPI communication) or write data to local files. Then call PMPI\_Finalize

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## Logging and Visualization Tools

- Upshot, Jumpshot, and MPE tools http://www.mcs.anl.gov/mpi/mpich
- Pallas VAMPIR
   http://www.pallas.com/
- Pablo <a href="http://www-pablo.cs.uiuc.edu/Projects/Pablo/pablo.html">http://www-pablo.cs.uiuc.edu/Projects/Pablo/pablo.html</a>
- Paragraph
   http://www.ncsa.uiuc.edu/Apps/MCS/ParaGraph/ParaGraph.ht
   ml
- Paradyn <a href="http://www.cs.wisc.edu/~paradyn">http://www.cs.wisc.edu/~paradyn</a>
- Many other vendor tools exist
  - e.g., xmpi (SGI and HP)

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## Future Opportunities in MPI Implementations

- I/O
  - Exploit MPI's sensible I/O semantics to get precise and latency tolerant behavior
- RMA
  - One-sided operations allow eager/ready-send behavior for messages of all sizes
- Dynamic processes
  - Major problem is the interaction with grid resource schedulers
- WAN Bandwidth
  - ◆ Multiple TCP paths (like GridFTP)
  - Customized UDP
    - May provide better congestion control, responsible sharing of bandwidth

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#### A Few Comments on I/O

- Applications with data at one location and compute resources at another may become a more common class of grid codes
- POSIX I/O requires very strong coherency
  - So strong that many systems don't provide POSIX semantics and instead provide ill-defined, cacheincoherent strategies
- MPI I/O has more precisely defined semantics that allow the MPI application to manage I/O sensibly (at least for a running MPI code)

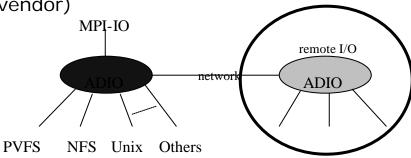
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### ROMIO -- A Portable Implementation of MPI-IO

- Implementation strategy: an abstract device for I/O (ADIO)
- Tested for low overhead
- Can use any MPI implementation (MPICH, vendor)



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#### Two-Phase Collective I/O

- ROMIO has an optimized implementation of two-phase collective I/O
- I/O is done in two phases: an I/O phase and a communication phase
- In the I/O phase, data is read/written in large chunks to minimize I/O latency
- Message-passing among compute nodes is used to redistribute data as needed

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#### Current State of MPI I/O

- Only prototypes exist for grid I/O
- On the other hand, very efficient cluster and MPP implementations exist
  - Short term recommendation
    - Use MPI I/O within a cluster and MPI communication to move data on the Grid
  - Long term
    - Expect (or contribute to!) the development of MPI I/O for the grid

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#### Fault Tolerance in MPI

- Can MPI be fault tolerant?
  - What does that mean?
- · Implementation vs. Specification
  - Work to be done on the implementations
  - Work to be done on the algorithms
    - Semantically meaningful and efficient collective operations
  - Use MPI at the correct level
    - Build libraries to encapsulate important programming paradigms
- (Following slides are joint work with Rusty Lusk)

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### Myths and Facts

Myth: MPI behavior is defined by its implementations.

**Fact:** MPI behavior is defined by the Standard Document at <a href="http://www.mpi-forum.org">http://www.mpi-forum.org</a>

Myth: MPI is not fault tolerant.

**Fact:** This statement is not well formed. Its truth depends on what it means, and one can't tell from the statement itself. More later.

Myth: All processes of MPI programs exit if any one process crashes.Fact: Sometimes they do; sometimes they don't; sometimes they should; sometimes they shouldn't. More later.

Myth: Fault tolerance means reliability.

Fact: These are completely different. Again, definitions are required.

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#### More Myths and Facts

Myth: Fault tolerance is independent of performance.

**Fact:** In general, no. Perhaps for some (weak) aspects, yes. Support for fault tolerance will negatively impact performance.

Myth: Fault tolerance is a property of the MPI standard (which it doesn't have.

Fact: Fault tolerance is not a property of the specification, so it can't not have it. ☺

Myth: Fault tolerance is a property of an MPI implementation (which most don't have).

**Fact:** Fault tolerance is a property of a program. Some implementations make it easier to write fault-tolerant programs than others do.

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## What is Fault Tolerance Anyway?

- A fault-tolerant program can "survive" (in some sense we need to discuss) a failure of the infrastructure (machine crash, network failure, etc.)
- This is not in general completely attainable. (What if all processes crash?)
- How much is recoverable depends on how much <u>state</u> the failed component holds at the time of the crash.
  - In many master-slave algorithms a slave holds a small amount of easily recoverable state (the most recent subproblem it received).
  - In most mesh algorithms a process may hold a large amount of difficult-to-recover state (data values for some portion of the grid/matrix).
  - Communication networks hold varying amount of state in communication buffers.

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## What Does the Standard Say About Errors?

- A set of errors is defined, to be returned by MPI functions if MPI\_ERRORS\_RETURN is set.
- · Implementations are allowed to extend this set.
- It is not required that subsequent operations work after an error is returned. (Or that they fail, either.)
- It may not be possible for an implementation to recover from some kinds of errors even enough to return an error code (and such implementations are conforming).
- Much is left to the implementation; some conforming implementations may return errors in situations where other conforming implementations abort. (See "quality of implementation" issue in the Standard.)
  - Implementations are allowed to trade performance against fault tolerance to meet the needs of their users

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## Some Approaches to Fault Tolerance in MPI Programs

- · Master-slave algorithms using intercommunicators
  - No change to existing MPI semantics
  - MPI intercommunicators generalize the well-understood two party model to groups of processes, allowing either the master or slave to be a parallel program optimized for performance.
- Checkpointing
  - In wide use now
  - Plain vs. fancy
  - MPI-IO can help make it efficient
- Extending MPI with some new objects in order to allow a wider class of fault-tolerant programs.
  - ◆ The "pseudo-communicator"
- Another approach: Change semantics of existing MPI functions
  - No longer MPI (semantics, not syntax, defines MPI)

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### A Fault-Tolerant MPI Master/Slave Program

- · Master process comes up alone first.
  - Size of MPI\_COMM\_WORLD = 1
- It creates slaves with MPI\_Comm\_spawn
  - Gets back an intercommunicator for each one
  - Sets MPI\_ERRORS\_RETURN on each
- Master communicates with each slave using its particular communicator
  - MPI\_Send/Recv to/from rank 0 in remote group
  - Master maintains state information to restart each subproblem in case of failure
- Master may start replacement slave with MPI\_Comm\_spawn
- Slaves may themselves be parallel
  - Size of MPI\_COMM\_WORLD > 1 on slaves
  - Allows programmer to control tradeoff between fault tolerance and performance

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#### State of Fault Tolerance

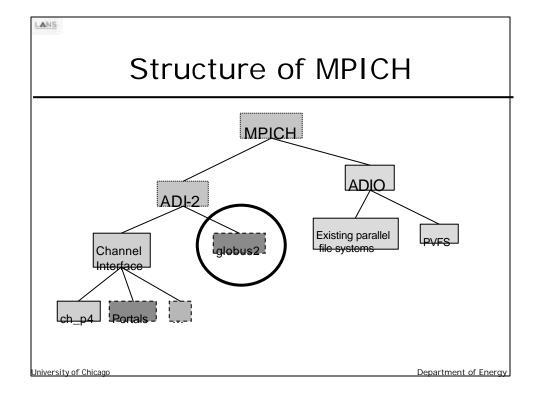
- Few MPI implementations are robust in the presence of communication failures (LAM/MPI can survive some)
- This should change in the next year

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## MPI Implementations for the Grid

- Use any cluster-based implementation
  - Rely on ssh or independently started, implementation specific demons to start processes
  - Issues are
    - · Executable distribution
    - Security
- Use IMPI
  - Only a few implementations
  - Simple security model
- Use an MPI implementation built on top of a solid Grid infrastructure
  - ♦ MPICH-G2

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#### What is MPICH-G2?

- Full implementation MPI 1.2 standard
- Developed by Nick Karonis (Northern Illinois University) and Brian Toonen (Argonne National Laboratory)
- MPICH-based, globus2 device
- Makes extensive use of Globus services, and therefore ...
- MPICH-G2 is a grid-enabled MPI

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#### Globus services in MPICH-G2

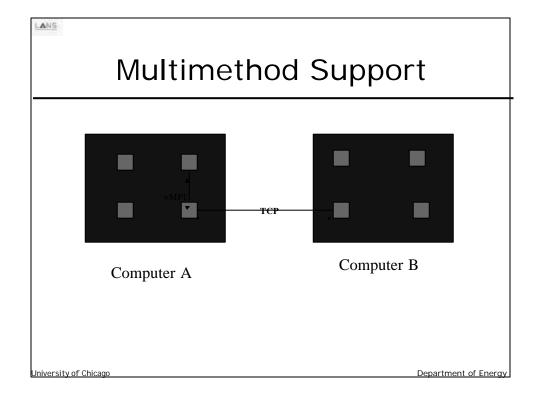
- Launching application
  - Resource Specification Language (RSL)
  - The Dynamically-Updated Request Online Coallocator (DUROC)
  - Globus Resource Allocation Manager (GRAM)
  - globusrun
  - Globus Security Infrastructure (GSI)
- Staging
  - Globus Access to Secondary Storage (GASS)
- TCP Messaging
  - Globus I/O
  - Data Conversion

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### MPICH-G2 is Topology Aware

- Topology-aware collective operations
- Topology-discovery mechanisms
- Topology-aware multimethod messaging

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## When should MPICH-G2 be used?

- Applications that are distributed by design
  - Scientific applications that need either more compute power, more memory, or both
- Applications that are distributed by nature
  - Remote visualization applications, client/server applications, etc.

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#### How to install MPICH-G2?

- Step 1 Install Globus
  - Acquire and install Globus v2.0 or later (http://www.globus.org).
  - Deploy a Globus gatekeeper (a demon) on each machine (not node!) you intend to run.
  - Acquire Globus identification (request from ca@globus.org) and set it up.
  - Add your Globus ID to Globus "gridmap" file on each machine you intend to run.
  - Test with "hello, world" program (from "Troubleshooting" section of www.globus.org/mpi).

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## How to install MPICH-G2? (cont.)

- Step 2 Install MPICH-G2
  - ◆ Acquire MPICH v1.2.4 or later.
  - ◆ setenv GLOBUS\_LOCATION to your Globus installation.
  - ◆ Pick a Globus "flavor" (never pick "threaded" flavor, always pick "mpi" flavor where available).
  - ◆ Configure MPICH with -device=globus2, make, make install

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#### How to use MPICH-G2?

- Step 1 Compiling your MPI application
  - source the file \$GLOBUS\_LOCATION/etc/globus-userenv.csh
  - ◆ Use MPICH-G2 compiler/linker:
    - <mpichpath>bin/mpicc
    - <mpichpath>bin/mpiCC
    - <mpichpath>bin/mpif77
    - <mpichpath>bin/mpif90

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## How to use MPICH-G2? (cont)

- Step 2 Running your MPI application
  - Use mpirun as described in manual, e.g.,

% mpirun -np 2 a.out arg1 arg2

#### Or

 Write your own Globus RSL script (www.globus.org) and supply that only

% mpirun -globusrsl myfile.rsl

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### Optional Execution-time Specifications

- Setting IP address range to specify a network interface
  - setenv MPICH\_GLOBUS2\_USE\_NETWORK\_INTERFACE <ipaddr>
- Setting TCP port range
  - setenv GLOBUS\_TCP\_PORT\_RANGE "min max"
- Request TCP buffer size
  - ◆ setenv MPICH\_GLOBUS2\_TCP\_BUFFER\_SIZE nbytes

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## MPICH-G2, Globus, and Firewalls

- It is possible to run MPICH-G2 applications through firewalls, but it takes sys admin cooperation.
- Described briefly, sys admins creates a small "hole" in the firewall called a controllable ephemeral port.
- You use GLOBUS\_TCP\_PORT\_RANGE to specify that port.
- For full dicussion of Globus and firewalls, see http://www.globus.org/security/v2.0/firewalls. html

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### Server Example

```
#include <stdio.h>
#include " mpi.h"

int main(int argc, char **argv)
{
    int passed_num, my_id;
    char port_name[MPI_MAX_PORT_NAME];
    MPI_Comm newcomm;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &my_id);
    passed_num = 111;

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```

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### Server Example (con't)

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### Client Example

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### Client Example (con't)

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#### Conclusions

- MPI the specification provides a good programming model for the Grid
- MPI implementations are usable, but more needs to be done
  - ◆ MPICH-G2: www.globus.org/mpi
- Many opportunities for both using MPI on the Grid and contributing to developing implementations that are "grid friendly"

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